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13. ABSTRACT (Maximum 200 words)
Accurate modeling and simulation of sensors is necessary to develop, test, and evaluate effective detection systems and decision support systems. The research performed in this Phase II SBIR contract developed a generalized architecture, framework, and methodology for the modeling and simulation of chemical and biological (CB) detectors. The software environment integrates atmospheric models, detector models, uncertainty measures, and a variety of time-synchronization and model composition capabilities. This framework provides distributed access to models and simulations. Simulation components were developed for standoff and point detectors, including the most complete dynamic model of the Surface Acoustic Wave (SAW) chemical sensor to date. The data resulting from the simulations enabled analysis of various detector capabilities and tradeoffs using multiple metrics.

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The investigators also acknowledge the assistance of the Defense Threat Reduction Agency (DTRA) (Ron Meris) and their contractors (Mark Quan of SAIC, Ron Lee of Oak Ridge National Laboratory) for the availability of HPAC and assistance in its preliminary integration.

The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or any agency thereof.

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1. Identification and Significance of the Problem or Opportunity

In the areas of chemical and biological defense, sensors play a critical role in providing data for the information fusion and decision support systems and their users. The input to decision support systems is the result of all the processes that occur from the source of the threat to the output of the sensors and associated detection systems. The output of sensors is determined by the chained sequence of processes, beginning at the threat source and propagating through the channel between the source and the sensor input. The detection system itself only imperfectly reproduces or classifies this distorted signal. The sensor fusion or decision support systems must interpret this imperfect data in a manner that provides accurate information to decision-makers. This research project developed tools to assist in modeling and understanding the behavior of chemical detection systems.

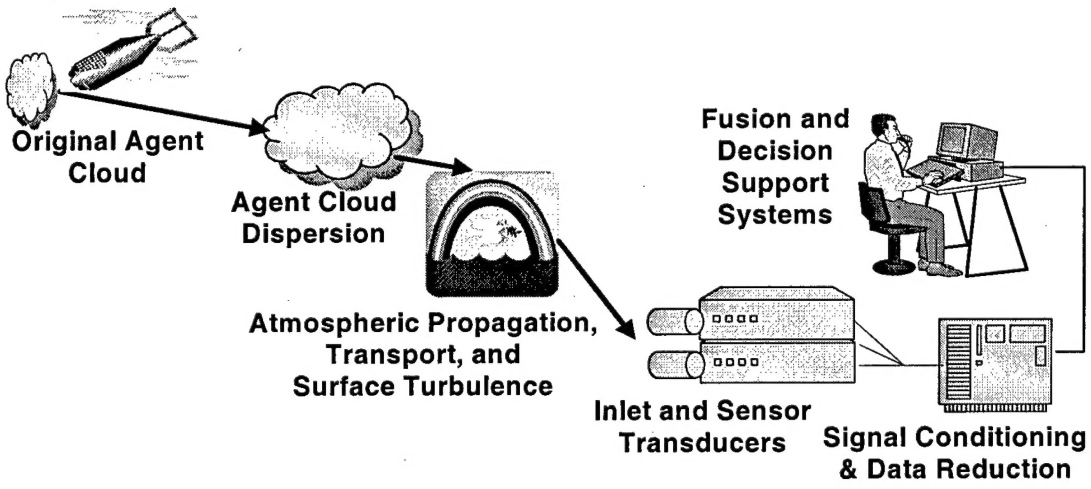

Figure 1. Information Flow from Source Cloud to Decision Support System

Figure 1 shows the flow of information from a chemical agent or simulation of an agent through other intermediate processes into a detection instrument. The input to the chemical/biological detection instruments must include the following sequence of processes or process simulations:

- agent source and initial agent distribution,
- agent transport and dispersion through the atmosphere,
- concentration fluctuations due to characteristic turbulence in the atmospheric mixing layer, planetary boundary layer, and near the inlet of a point detector,
- distortions caused by transport of matter or radiation to the transducer sensor component that converts either the radiation or chemical inlet to an electrical output,
- the method of signal transduction and associated electronic signal conditioning,
- the effects of interferent chemical species as well as interfering ambient and jamming radiation on sensor signal transduction,
- data reduction algorithms for both signal and intrinsic noise, and
- the algorithms that translate the digitized electrical signals or spectra into information on agent concentration, type and distribution.

The outputs from this sequence form the inputs to detection instrument data fusion and C4I decision support systems. The output of the detector/sensor is not the information being sought by commander decision support systems; rather, these decision support systems require accurate reproduction of the sensor inputs and environmental conditions.

1.1. Survey of Chemical Detection Systems

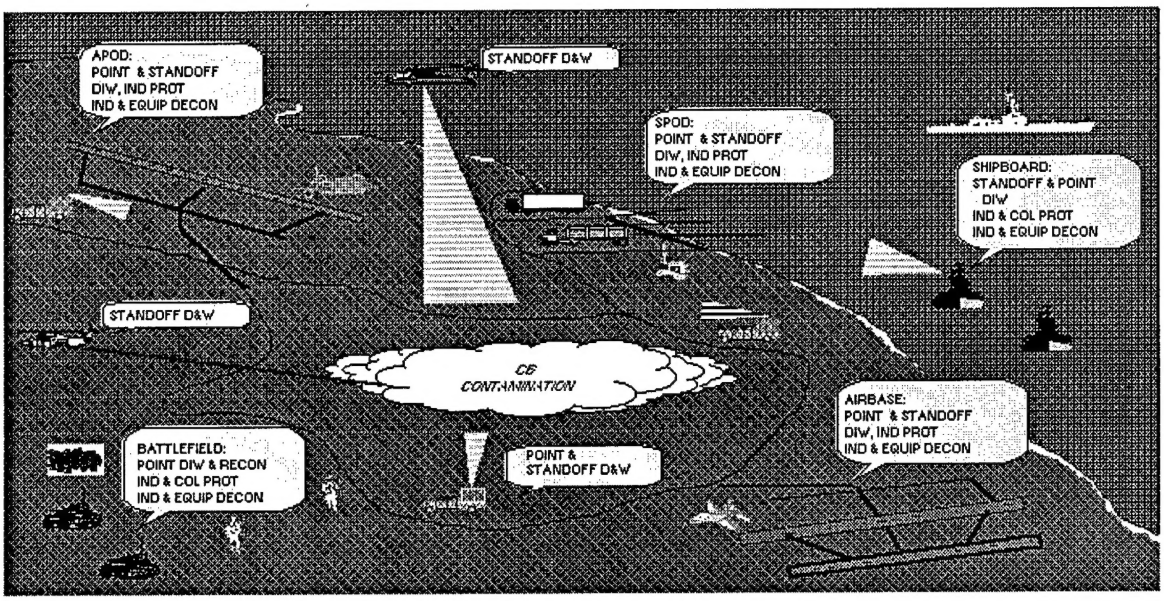

Figure 2. Sensors and Decision Support in Battlefield C4I using a Chem./Bio Scenario (US Department of Defense, 1997)

Figure 2 shows common sources of sensor data in a chem./bio defense scenario. Decision support systems for Chemical and Biological Defense (CBD) rely heavily on both raw and transformed sensor data. Chemical and biological detection systems incorporate a variety of physical sensors. A chem/bio sensor is a transducer, which represents the concentration of toxic agents by transforming a physically measured property to an electrical output.

Point detectors transform in situ chemical concentrations to an output current or voltage. Point detectors take samples of the atmosphere that interacts with the sensor, sometimes after a separation technique. Many interaction mechanisms are possible, but all of them result in either charge generation or changes in electrical potential. Examples include ion mobility spectrometry, surface acoustic wave techniques, flame photometry, catalyst coated solid polymer electrolyte devices, and various surfaces or solutions coated with bioactive organisms or compounds.

Standoff detectors transform the complex emission, absorption, reflection and propagation of electromagnetic signals through the atmosphere into an electrical output pattern. The two main types of standoff detectors are passive and active. Passive standoff detectors measure the radiation incident on a detector from the atmosphere using ambient light to serve as the light source. In these systems, the detectors capture the composite spectra of many atmospheric

gases. Both active and passive detection involves separating the spectra of benign and background gases from potentially toxic components of the atmosphere.

Active standoff detection systems generate an electromagnetic wave at the source (e.g., laser, Xe-arc lamp) and then detect the returned wave using an optical receiver (e.g., optics, beam splitting lenses and mirrors, optical detectors). The delayed, attenuated and phase-shifted return signal is matched against the expected return signal in the presence or absence of a toxic agent. A high fidelity atmospheric model is needed to provide baseline wave propagation predictions and enable the subsequent creation of pattern recognition algorithms to identify the constituent chemicals. A prominent form of active standoff detector is an infrared optical radar, commonly known as Light Detection and Ranging (LIDAR). Chemical identification of toxic agents in clouds is enhanced by using dual wavelength, dual beam sources in a form of LIDAR known as Differential Absorption LIDAR (DIAL).

Each type of sensor has different input/output characteristics and operates through different physical mechanisms. The impact and effects of environmental processes on the detection system will depend on the specific mechanisms of each detection process. However, all detection systems will be influenced by common atmospheric properties and processes, including the presence of interferents, thermodynamics and physical properties, agent transport and dispersion, and environmental turbulence characteristics. Many of the inputs to the detection systems result from stochastic processes, and observations contain uncertainty at various levels of the detection process. In many cases, detection systems will need to fuse data from multiple types of sensors and associated interpretation algorithms to provide more robust identification and quantification of toxic agents in the environment.

In principal, the point, active standoff, and passive standoff detection techniques can effectively detect chemical/biological agents. In practice, the detectors do not exhibit ideal behavior and their inputs in the natural environment (e.g., stochastic processes) deviate substantially from those used in typical laboratory tests. Point detectors are typically used for alerting and alarming personnel in the immediate area to the existence of toxic compounds. The observation point may or may not be representative of the immediate surrounding area or the larger battle area. For this reason, point detectors are deployed in arrays or mobile platforms. Because standoff detectors provide spatially averaged data concerning the existence and concentration of agents, they are most commonly used for identifying threat clouds and alerting field personnel to an incipient threat.

1.2. Significance of Accurate Modeling of Chemical and Biological Detection Systems

There are challenges and deficiencies in current detection technologies and their deployment, such as high false alarm rates, sensitivity to interferents, suboptimal data interpretation algorithms, and inability to adapt to new threats. The effectiveness of chem/bio detection, information fusion, and decision support systems depends greatly on their ability to incorporate sophisticated and accurate information, such as expected detector performance under various conditions, ranges of realistic operational conditions/limitations, and meaningful representations of uncertainties and effects arising from environmental conditions. DoD and DHS platforms in the areas of hazard prediction/assessment (e.g., JEM, DTRA HPAC, JWARN), detector

design/deployment, and consequence management would benefit from an integrated solution that accurately simulates sensors, detection systems, and arrays of detection systems under realistic conditions.

Accurate modeling and simulating the behavior of detection systems under real-world conditions can aid the design, development, and test of detection systems themselves and other systems that operate upon their data. Other existing CB sensor modeling, simulation and acquisition environments do not accurately predict CB detector performance under realistic battlespace conditions. For example, some DoD training systems utilize a lookup table of prerecorded field data observations of the detection systems. Field test data, including data collected at U.S. Army Dugway Proving Ground, is critical for the verification and validation of sensor models and simulations. While real field data on sensor performance can be collected at test ranges, the results do not necessarily predict the performance of that instrument in different locations and operating conditions (e.g., Winter in Afghanistan or Summer in Iraq). The predictive power of real field data is limited because they can only span a very limited portion of the mission space of the detector. Therefore, while field data may be useful for some training systems, this approach can not meet the requirement to predict future behaviors.

The chem/bio simulations should incorporate a combination of chemical/physical and empirical models, their associated uncertainties, and realistic conditions. These accurate models and simulations of decision support input data from sensors and other sources enable effective development, test, and evaluation and use of decision support systems. In order to predict an output of a sensor system under any arbitrary conditions within its mission space, a complete dynamic (time varying) model is required. Empirical models determine their parameters from data (e.g., scene generator data, experimental detector data, simulation data from atmospheric models) and performance measures that characterize a system over its entire mission space. Therefore, dynamic models and simulations valid over the entire mission space are needed to provide sensor output data that facilitates the design of decision support systems effective over a full range of battlefield situations.

1.3. Need for a Comprehensive Detection Systems Simulation Architecture and Framework

The utilization of high fidelity, dynamic chemical detection models can increase the efficiency and reduce the time to design, develop, test, and refine chemical detection systems and information fusion systems. A single monolithic model capturing all of the behaviors of a given sensor or sensor suite would be inflexible, difficult to maintain, and computationally inefficient. Likewise, a collection of high quality models of different aspects of the detection process would be most useful if the results of one simulation is available as the input to another, in real-time. For the user community to realize the potential of simulation-based acquisition, design, and test, the users need a software architecture that enables them to integrate models from various sources, modify these models, validate them, and use them for the purposes of design, test, and analysis.

An environment which permits the flexible authoring and assembly of sensor/detection system components, along with their associated uncertainties, would enable the stakeholders to effectively reuse simulation resources and rapidly test a variety of scenarios and optimization

criteria. Composability is "the capacity to select and assemble simulation components in various combinations into simulation systems for different purposes" (Petty and Weisel, 2003). The benefits of composability include more comprehensive simulations, the ability to enforce consistent assumptions, increased validity, and more efficient and responsive use of resources (Kasputis and Ng, 2000). In a sensor simulation environment, composability would facilitate the creation, maintenance, and reuse of libraries of sensor/detection simulation components optimized for various fidelities, scenarios, and assumptions. Simulation software developers, modelers, integrators, testers, and users require the ability to rapidly and flexibly develop and compose new components and simulations to satisfy the specific needs of the user. This will require the rapid configuration, verification, validation and deployment of these components.

There are several initiatives in the simulation community for the creation of composable simulation environments, including the eXtensible Modeling and Simulation Framework (XMSF) initiative (Brutzman, 2003), the SISO Base Object Model (BOM) Product Development Group effort (Simventions, 2005), and the Simulation Reference Markup Language (SRML). In the efforts by the SISO BOM PDG, a BOM represents information (e.g., metadata) about a single simulation federate, represented in XML. The SISO BOM PDG is developing standards for BOMs that will enable simulation interoperability, reusability, and composability. The eXtensible Modeling and Simulation Framework (XMSF) is an initiative to define a set of web-based technologies to support interoperability among Modeling & Simulation (M&S) applications (Brutzman, 2003). The Simulation Reference Markup Language (SRML), submitted by Boeing to W3C, describes some basic metadata for simulation BOMs in XML, as well as additional functionality for representing behavior (e.g., scripting capabilities) (Reichenthal, 2003; Boeing, 2003). These efforts complement the research described in this report.

1.4. Software Implementations of a Sensor Simulation Environment

At present, an integrated solution, including source code Integrated Development Environment (IDE), visual composition environment, source code and version management, management of various simulation resources, and domain-specific libraries, does not exist for chem/bio detection simulations. However, several Department of Defense contractors have developed systems that have a predefined library of chem/bio sensor models and interfaces to DoD standards. These systems readily integrate with existing DoD simulation standards and have been successfully deployed for some applications (e.g., training, battlefield scenario assessment).

Many of these chem/bio detection simulation environments incorporate simplistic or inaccurate chem/bio detection systems models, leading to suboptimal allocation of resources and reduced probability of mission success. For example, many of these simulation environments do not incorporate realistic physico-chemical models, are not typically capable of predicting real-world outputs under the time varying or turbulent conditions expected in the battlespace or homeland, and do not incorporate relevant forms of uncertainty (e.g., stochastic processes, numerical precision, etc.).

In addition to the more proprietary chem/bio simulation offerings, there are also general-purpose commercial-off-the-shelf (COTS) environments for simulation and simulation development.

Among the most widely used and respected is Mathworks Simulink® which provides a toolset for modeling, simulating, and analyzing dynamic multi-domain systems.

1.5. Benefits

Many existing CBD decision support systems will benefit from the incorporation of more accurate understanding and description of the outputs of the sensor components of detection systems. At present, DTRA HPAC and JEM have high quality decision support, casualty prediction, and atmospheric modeling capabilities to support chemical/biological defense. Simulation developers, detection systems designers, decision support system developers, and other decision makers within various DoD test and evaluation facilities need a comprehensive tool that integrates atmospheric models, chem/bio detector models, and information fusion/decision support systems. For example, decision support systems such JWARN and Army Future Combat Systems would benefit from working with realistic representations of detector responses.

Modeling the behavior of the sensor or detection systems would also enable the development, test, evaluation, and effective utilization of sensor interpretation and fusion algorithms that address these issues. These models would also enable the optimization of system performance by alteration in detection hardware and software system architecture, components, and parameters.

The prototype developed in this research enables the development, integration, execution, and analysis of models that accurately predict sensor performance. While this may expose previously unanticipated limitations, it will also provide defensible and believable predictions of operational performance for the ultimate users, the military in the field. In this research, the investigators focused on demonstrations of models of chemical and biological (CB) detectors as the problem of CB detection represents a still unsolved challenge for homeland and military defense and response. However, the technologies could be applied to other sensor modeling domains in the future.

2. Technical Objectives for the Phase II Research

- A Visual Simulation Composition Environment including
  - The ability to visually create models and run simulations composed from components, which are visually represented on a pallette
  - Support for nested, coupled models
  - Configuration of time policies for individual simulations and coupled simulations
  - Data visualization
- A simulation engine and associated repository that supports
  - A framework support for nested, coupled simulations
  - Time Synchronization for coupled dynamic simulations
- Integration of atmospheric models
  - Preliminary integration of HPAC through its CORBA interface
- Resource Management
- Integrated Development Environment for simulation source code
- Source code management & development
- Resource versioning & management
- Uncertainty representation and propagation

- Libraries of performance metrics
- Representations of uncertainty for different classes of algorithms
- Propagation of uncertainty across coupled simulations

- Software Interfaces for components to
- Source code / executable code
- Distributed objects (e.g., CORBA-compliant objects)
- Composite models
- Implementation and integration of models
  - A repository of primitive composable models useful for constructing more complex simulations
  - Artemis CB standoff detector models
  - Surface Acoustic Wave (SAW) models developed by the University of Utah

3. Software Architecture

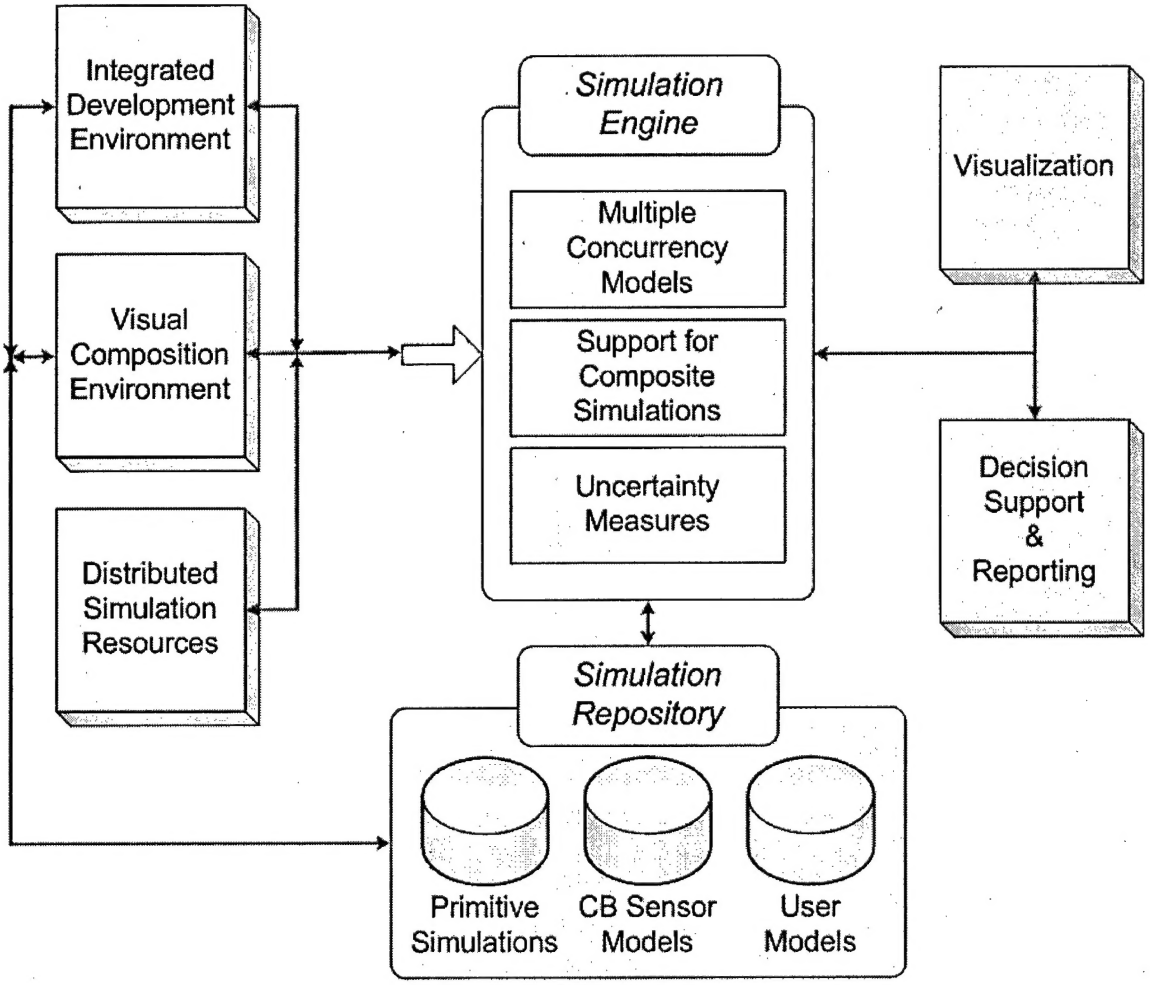

Figure 3. Overall Architecture of the Sensor Simulation Environment

4. Selection of Core Technologies

At the beginning of the Phase II effort, the investigators identified and evaluated several available core technologies for the Phase II simulation framework, which enabled the development of the software implementation. The investigators began the integration of core technologies, such as the Eclipse open source Integrated Development Environment (IDE) framework and Ptolemy heterogeneous concurrent modeling framework, within the Phase II software framework. Because the core components of the environment are written in the Java programming language, it can operate on a variety of hardware and software environments. All C and C++ development is compatible with the GNU gcc compiler suite that is also openly available on a variety of platforms. The integration of these technologies provided an extensible and configurable simulation development, testing, integration, and evaluation environment. Furthermore, these technologies provide other capabilities (e.g., MatLab integration, software development tools, resource management tools) that directly benefit the ultimate product.

4.1. Eclipse

The Eclipse project is an open source framework designed to provide a commercial-quality platform for highly integrated tools (Eclipse Foundation, 2005). The project was started when IBM released approximately $40 million of developed software as open source technologies. Eclipse is a cross-platform framework, already supported by several high-quality tool plug-ins:

- JDT, an open source Java integrated development environment (IDE);
- CDT, an open source C/C++ IDE;
- Open source resource management tools (i.e., Team/CVS, Stellation);
- Commercial embedded development tools (e.g., QNX);
- Data modeling tools from database vendors (e.g., Oracle, Sybase); and
- Rational™ modeling and software life cycle tools.

Although Eclipse is a relatively new technology, there is a lot of commercial support from a number of companies including IBM, RedHat, QNX, and SyBase allowing a large amount of responsiveness to the needs of developers using the framework.

By integrating the sensor simulation framework within Eclipse, the researchers would be able to provide an integrated platform for simulation development, testing, execution and analysis. The Eclipse framework will also allow the researchers to provide wizards and templates to increase the usability of the APIs. The Eclipse framework enables different utilities and tools to be configured into customized services according to user roles and tasks.

4.2. Ptolemy

Ptolemy (University of California, 2003), a research project at the Department of Electrical Engineering and Computer Science at the University of California Berkeley, studies heterogeneous modeling, simulation and design of concurrent systems. Its research and associated development has been supported over the last ten years under contracts with DARPA, NSF, and various commercial partners. The focus of their research is on embedded systems, particularly those that mix technologies including analog and digital electronics, hardware and software, and electronics and mechanical devices. They also focus on systems that mix widely different operations such as signal processing, feedback control, sequential decision making and user interfaces.

The Ptolemy project is driven by the principle that the choices of models of computation strongly impact the quality of a system design. This led to the development of a library of tools capable of combining different choices of computation management including discrete event, discrete time, continuous time, synchronous data flow, and finite state machines.

In addition to the abstractions in computational techniques and the inherent support for nested and coupled dynamic simulations, Ptolemy also offers a dynamic typing system in the Java programming language. Ptolemy's dynamic type system and Java implementation were developed by Yuhong Xiong as part of his Ph.D. thesis from U.C. Berkeley. The type system leverages algorithms from the ML software language and allows run-time type checking and lossless hierarchical type conversion. CogniTech leveraged and extended this type framework to express the different measures of uncertainty required for this effort.

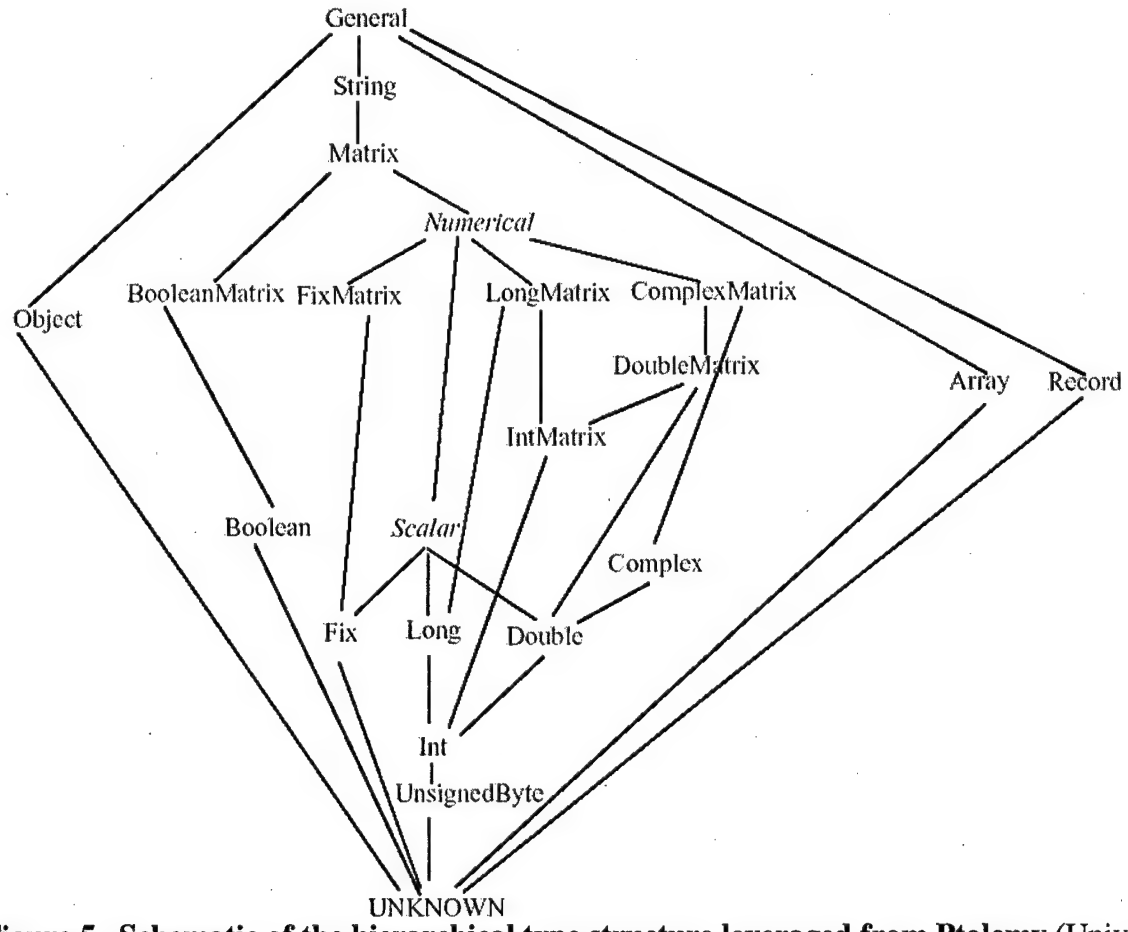

Figure 5. Schematic of the hierarchical type structure leveraged from Ptolemy (University of California, 2003)

5. Development of Simulation Framework

The investigators developed a simulation framework that combines Ptolemy's simulation engine and visual composition environment, extensions to handle uncertainty, Eclipse's source code / resource management capabilities, and additional models to support CB detection modeling. All

programming was done in the Java programming language. The Ptolemy simulation framework enables the composition of simulations containing different or hybrid models of computation, including discrete event, discrete time, continuous time, synchronous data flow, and finite state machines.

The CogniTech sensor simulation environment enables the full life cycle of simulation design, development, integration, test, deployment, analysis, and maintenance. It includes an Integrated Development Environment (IDE), visual composition environment, source code / version management, management of various simulation resources, and domain-specific libraries, to develop chem/bio detection simulations.

Table 1. Current Capabilities of CogniTech's Sensor Simulation Environment

FEATURE	ADVANTAGE	BENEFIT
Run-time implementation	Hierarchical composition of simulations	Simulation environment solves complex problems and supports iterative model refinement
Uncertainty representations	Manages representation, propagation & visualization of uncertainty	Can incorporate & analyze uncertainties for process / system
Visual composition environment	Palette of components for visual composition & creation of new components	Create new components & rapidly use components to create complex, composite simulations
Role / User configurable Workspace	Allows customized user's workspace	Increased user productivity
Visualization tools	Provide capability to graph & display data	Visually display simulation results
Source code management & development	Capabilities to manage Java & C/C++ simulation source code	More time & cost-effective development efforts
Resource versioning & management	Manage other forms of simulation resources	Multiple users can search for & manage versions of resources
Distributed Software Interface	Prototype for CORBA interoperability. Plans for HLA and BOM interoperability (not implemented in Phase II).	Interoperable with legacy and future software that uses these distributed communications standards

Detailed features and comparison with Mathworks Simulink® are presented below.

Features/Benefits	CogniTech	Simulink®
Visual Composition Environment	✓	✓
Matlab Integration	✓	✓
Programming Language Interfaces	✓	✓
Integrated Debugger	✓	✓
Uncertainty Measures and Metrics	✓+	✓-
Multiple Concurrency Models	✓+	✓-
Source code and version management	✓	
HLA (Planned) and CORBA (Proof-of-Concept) Integration	✓-	
HPAC Integration (Proof-of-Concept)	✓-	
Open API	✓	
Libraries for Chem/Bio Simulation	✓	

Table 2. Comparison of Current CogniTech Environment and Mathworks Simulink®

Within the sensor simulation environment, simulations can initially be developed or integrated at either the source code level or through the use of a graphical editor to visually wire simulation components (primitive simulation units or more complex nested components) together. The graphical simulation editor stores the simulation information including simulation components and their connections, scheduling information, and user specified parameters in the form of an XML file which is submitted to the simulation engine for execution. Simulation components can be simulation source code, executable libraries, or components that are composed from these primitive simulation units. Components available from the repository appear on a palette, available to support the user's visual construction of more complex simulations and simulation components.

5.1. XML Editor

Leveraging existing open source tools, CogniTech developed an XML editor including simplified syntax highlighting and formatting which was integrated into the environment. This editor was then registered for file type association within the workspace allowing automated execution of the editor when opening the file similar to the file association familiar from operating systems. Although the editor is not "DTD aware" and does not provide automated markup of higher order data structures within the XML, it is sufficient for present use and will be developed further based on project needs and following an initial end to end implementation of the environment's required functionality.

5.2. Simulation Graph Editor / Visual Composition Environment

CogniTech is leveraging the Vergil graphical simulation editor from the University of California, Berkeley Ptolemy project. CogniTech has begun the integration of this tool into the Sensor Simulation Workspace. This effort aligned both graphical and Model View Control abstractions between the workspace and Vergil. Although sections of the original Vergil source code are modified, CogniTech localized source code changes and minimized their footprint to enable the seamless integration of future Vergil releases into the Sensor Simulation Environment.

5.3. Simulation Resources, Repository and Simulation Execution

After the graphical construction of a simulation from components, the simulation can be submitted to the Simulation Engine for execution. The Simulation Engine will manage the execution of the defined components and the output/storage of the data. The Simulation Engine coordinates the execution of the following simulation resources:

- components bundled with the initial installation;
- components dynamically linked from within the user's workspace, and
- components installed as libraries following initial installation.

5.4. Uncertainty Management

A major focus of CogniTech's Phase II research was the ability to characterize the different types of uncertainties within a simulation and simulation components. As discussed within previous reports, there are numerous sources and types of uncertainty within sensor and CB sensor simulations. CogniTech has begun the implementation of abstract data types for using internal uncertainty representations within a simulation. Classical statistical measures and their

associated operations are supported within the environment. In addition, the simulation environment provides the ability to be extended to support additional measures and their operations. Interval measures were chosen for the initial implementation because they are computationally well defined and provide a useful basis for initial uncertainty representations.

There are many sources of uncertainty that can impact a computational modeling result. There are uncertainties in model parameters and experimental data used by a computational model. Since computational models must use the finite set of floating-point numbers that the hardware makes available, there are uncertainties associated with round-off, truncation, approximated mathematical functions and other operations. Interval mathematics provides a relatively simple way to quantify such uncertainties. Interval mathematics is a generalization of real mathematics that uses two floating-point numbers to bound the uncertainty associated with each real number. Interval arithmetic (Alefeld, 1983) can protect the correctness of results against uncertain data, rounding errors, and inexact algorithms.

As an example of interval computing, suppose we wish to add the uncertain parameter $\alpha = 3.2$ to the uncertain parameter $\beta = 7.3$. We are very confident that α is known to within 0.3 units, and β is known to within 0.2 units. Using this information, we can construct the corresponding intervals

$$\alpha \equiv [\alpha - 0.3, \alpha + 0.3]$$

and

$$\beta \equiv [\beta - 0.2, \beta + 0.2].$$

Therefore, the results of adding these values are

$$\alpha + \beta = [2.9, 3.5] + [7.1, 7.5] = [10.0, 11.0].$$

According to the operations of interval arithmetic, the resulting interval is calculated by

$$2.9 + 7.1 = 10.0$$

and

$$3.5 + 7.5 = 11.0.$$

Therefore, rather than a simple approximation to the result $\alpha + \beta$, we have a reliable conclusion that the true solution is within the produced bounds, despite uncertain data, finite precision, and approximation.

The process of propagating intervals throughout the entire computation guarantees that the result of the interval computation is contained within the resulting interval. Given the simplicity, elegance, and utility of interval mathematics, this was the initial form of uncertainty added to the simulation framework.

5.5 An Overview of Current Capabilities

The distribution includes a sample project with a number of example simulations using different synchronization strategies. The examples project may be accessed by following these steps, as shown in Figure 6:

- File>Import>Existing Project Into Workspace and
- browsing to and selecting the Examples directory under the installed workspace.

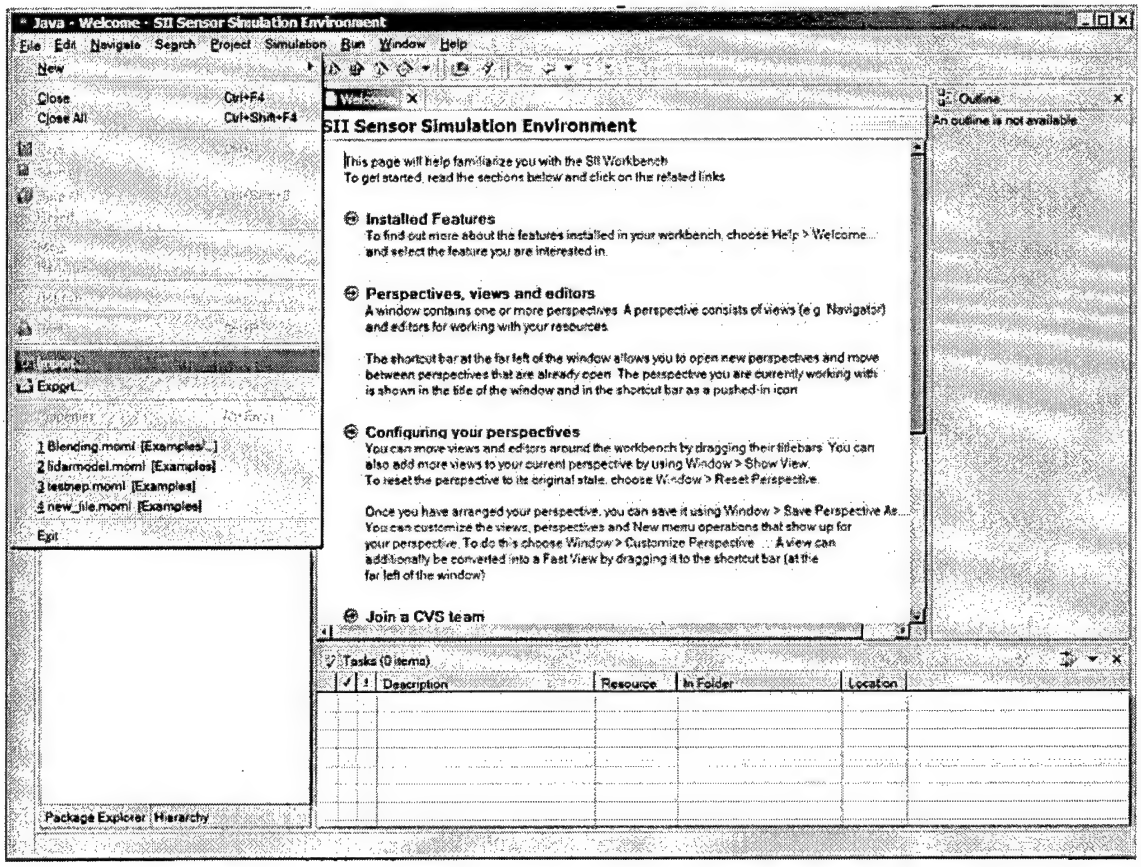

Figure 6. Importing the Example Project.

Figure 7 shows the main workspace window of the simulation IDE. The leftmost panel is a resource explorer. Different resource explorers are available with different types of filtering based on resource type and the type of project. In this case, the user has one project within their workspace. Each project has a specific nature associated with it that defines the default editors and information viewers when accessing the project. Within the "ChemBio Simulations" project, the user has several .moml simulation files that describe the composition of the simulation components and synchronization strategy.

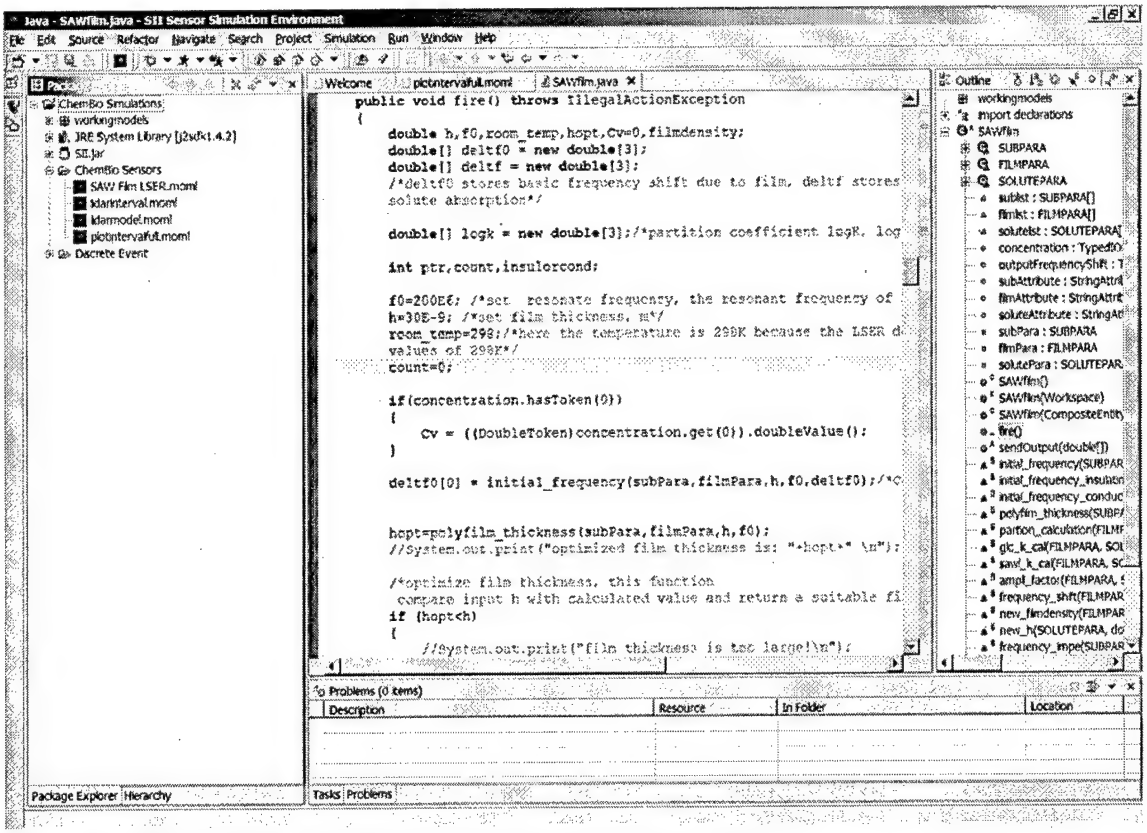

Figure 7. Simulation Workspace with Source Code View

In the top center panel of Figure 7, the workspace contains a Java Editor for the source code of a simulation unit. In this case it is the source code of a model simulating the behavior of a Surface Acoustic Wave sensor.

Below the Java editor, notice the Task Window. By default, this will list compiler warnings and errors. When a user double clicks on an entry in the Task Window, the appropriate editor opens and brings focus to the appropriate location in the file. The user can also configure the workspace to use custom keywords such as "TODO" as a task flag. Users of the simulation workspace can drag-and-drop or resize different views (e.g., source code, hierarchy, resources) of simulation components into a persistent customized workspace configuration.

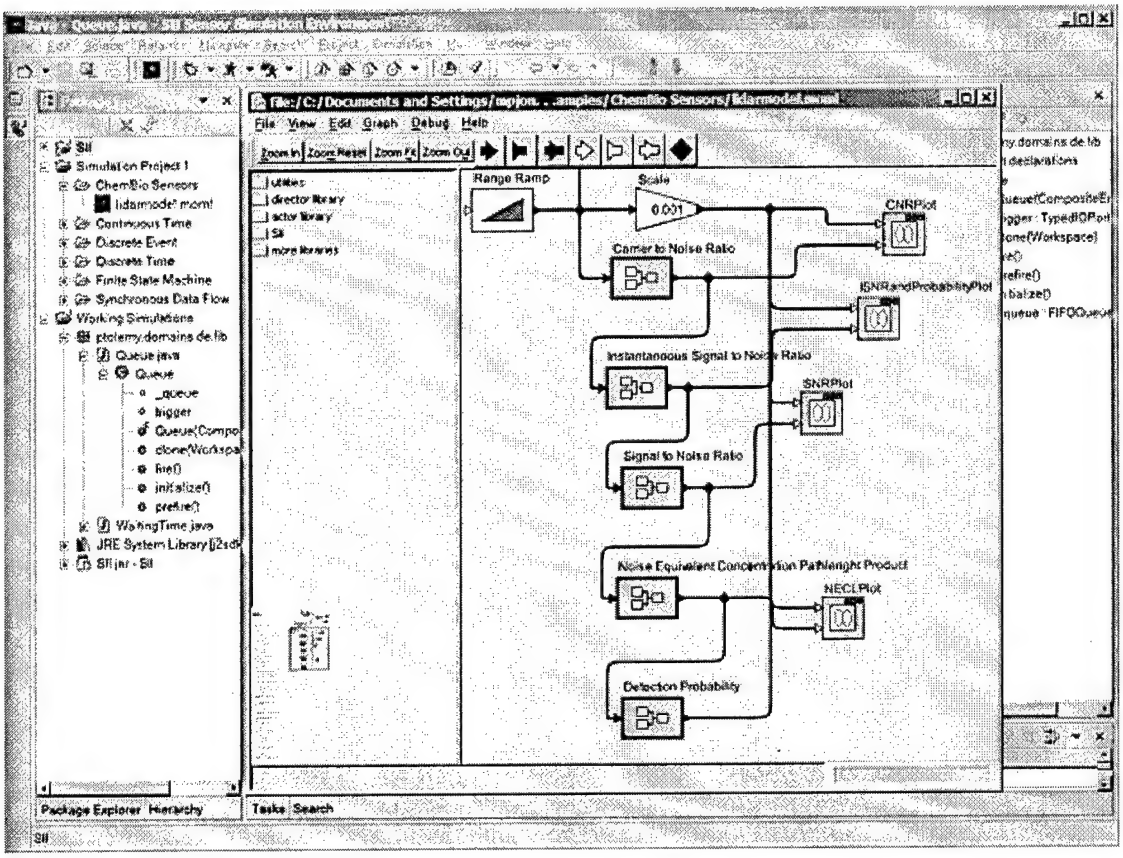

Figure 8. Simulation Environment with open Simulation Graph Editor

When an MOML XML file is opened within the workspace, a Simulation Graph Editor (as shown in Figure 8 above) is automatically launched. On the left side of the Simulation Graph Editor, the Repository Palette contains reusable simulation components that may be dragged and dropped to perform simulation wiring and other simulation construction tasks. Below the Repository Palette, a navigation window allows the user to easily move the focus of the main Graph Editor pane. Within the main Graph Editor pane, the simulation is visually constructed. Each simulation contains a Director which manages the synchronization between components. Different Director's are available for different synchronization schemes (discrete event, continuous time, etc.).

The model in Figure 8 shows an example of a graphically composed LIDAR model that determines the detection probability of an agent based on various parameters including species absorption wavelength and range. Components within the editor using the icon are nested simulations each with their own Director and synchronization strategy. Figure 9 shows the internal construction of one of these sub-models.

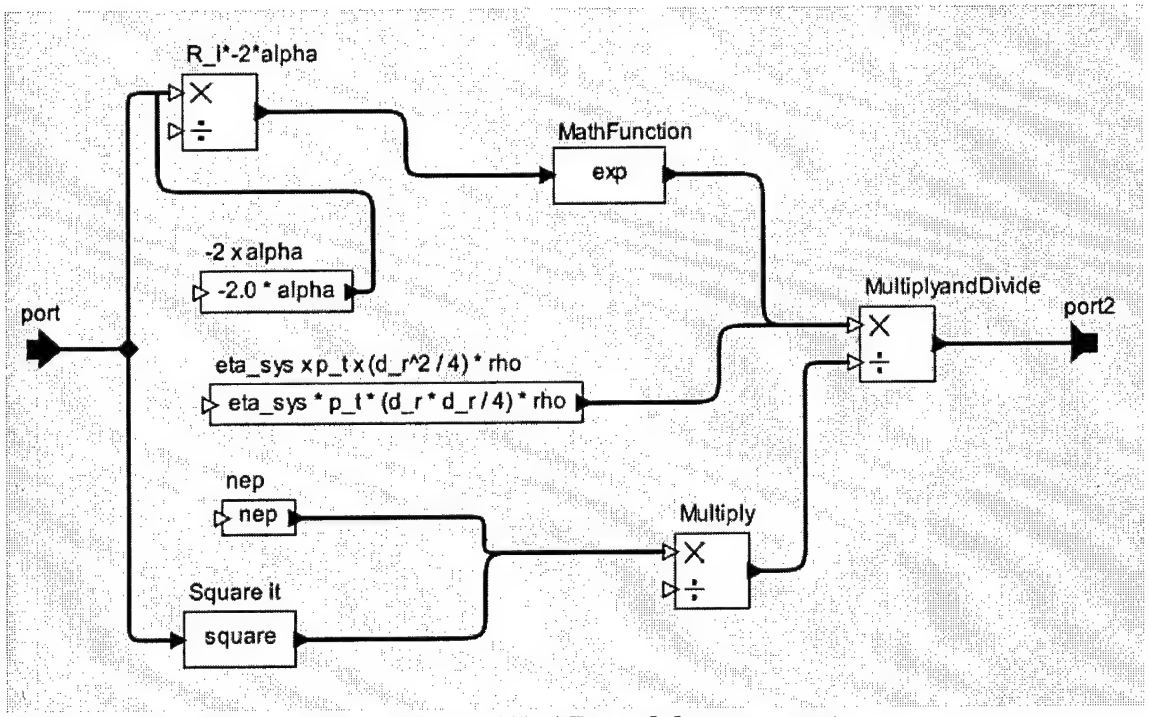

Figure 9. Visually composed nested LIDAR model component

Individual models are opened by double clicking on the "moml" file. The Run Window is accessed from the Graphical Simulation Editor by following these steps:

- View>Run Window and
- Clicking the "Go" button begins execution.

The data resulting from running a simulation can be presented to the using through visualization capabilities.

5.6 Visualization

The simulation environment provides the ability to plot and chart simulation data and view the evolution of these plots in real time as the simulation evolves. In addition, the simulation environment provides an API for the development of custom visualizations including animations that leverages Sun Microsystems Java Imaging library.

In addition to basic visualization capabilities, specific visualization tools were developed to support the Phase II research. After interval measures for uncertainty were added as a basic data type for the simulation framework, the investigators decide to add custom visualization tools to represent this form of uncertainty. The existing visualization utilities were augmented to display the span of an interval measure within a graph. Figure 10 in section 6.3 illustrates an example of visualization for data from a LIDAR simulation.

6. Model Development and Analysis

One of the most significant contributions of this research was recasting mathematical representations/models of the operating mechanisms for point and standoff detectors. This was demonstrated using two models of chemical detectors: a baseline model of a LIDAR standoff detection system and an in-depth model of a SAW chemical point detector.

6.1. LIDAR Models

6.1.1. Overview of LIDAR Systems

Active standoff detection using differential absorption lidar (DIAL) is an ongoing area of research for atmospheric chemical detection and systems using a wide number of different measurement and analysis techniques have been developed. DIAL systems provide the ability for three-dimensional mapping, identification and quantification of chemical species' concentration profiles within the atmosphere. To accomplish this, laser light is transmitted into the atmosphere at two similar wavelengths. One wavelength is chosen at which the species under investigation absorbs the light and the second is a near (off peak) wavelength. If the two pulses are made close enough in time such that the atmosphere can be considered stationary, the off peak laser pulse is assumed to have similar atmospheric transmission characteristics to the on peak wavelength except for optical absorption by the chemical species. Comparison of the intensities of the backscattered pulses given the concentration of the investigated species in the region of atmosphere examined. Range is determined by resolving the arrival time of the returning pulses.

6.1.2. DoD LIDAR Model

To demonstrate the present capabilities of the sensor simulation environment, CogniTech used simplified LIDAR model obtained from the Artemis program was implemented within the sensor simulation environment. Within the sensor simulation environment, users, at present, may chose one of two methods for implementing simulations. First, the sensor simulation environment provides a repository of useful simulation components (Atomic Actors) that may be wired visually to construct a composite simulation. In addition, users may otherwise opt to develop component simulations leveraging the existing software API and libraries.

For demonstration purposes, the Artemis LIDAR model was implemented using primitive simulation units available within this distribution. Since model components only rely on incoming data on which to operate, the Synchronous Dataflow director was chosen for both implementations.

The Artemis LIDAR model has sixteen adjustable parameters. From these parameters, the model predicts the probability of direct detection

- noise power and plots the following versus range;
- carrier to nose ratio;
- signal to noise ratio;
- instantaneous signal to noise ratio; and
- probability of detection.

The LIDAR model was implemented with nested models for the noise power, carrier to noise ratio, signal to noise ratio, and probability of detection.

6.1.3. Analysis of LIDAR Simulation and Uncertainty

Figure 10 shows the results of the probability of detection LIDAR simulation for both expected and numerically uncertain outputs. The bottom portion of this figure shows the result from introducing small uncertainties in the detection threshold and false alarm rate parameters. The

interval, representing uncertainty in the detection probability curve, is represented by error bars on a discrete sampling of points. For clarity, the entire probability of detection curve is not plotted. Through the use of interval mathematics, these uncertainties were propagated throughout the model calculations to produce the intervals shown in the lower half of this figure. The utility of interval mathematics is its ability to provide insight into how uncertainty of selected parameters may impact uncertainty associated with a system. The top part of the figure suggests that the probability of detection is near one up to about nine km. Between nine and eleven km, the probability transitions to zero. The lower plot shows sensitivity to uncertainty in the region between nine and eleven km, indicated by larger error bars.

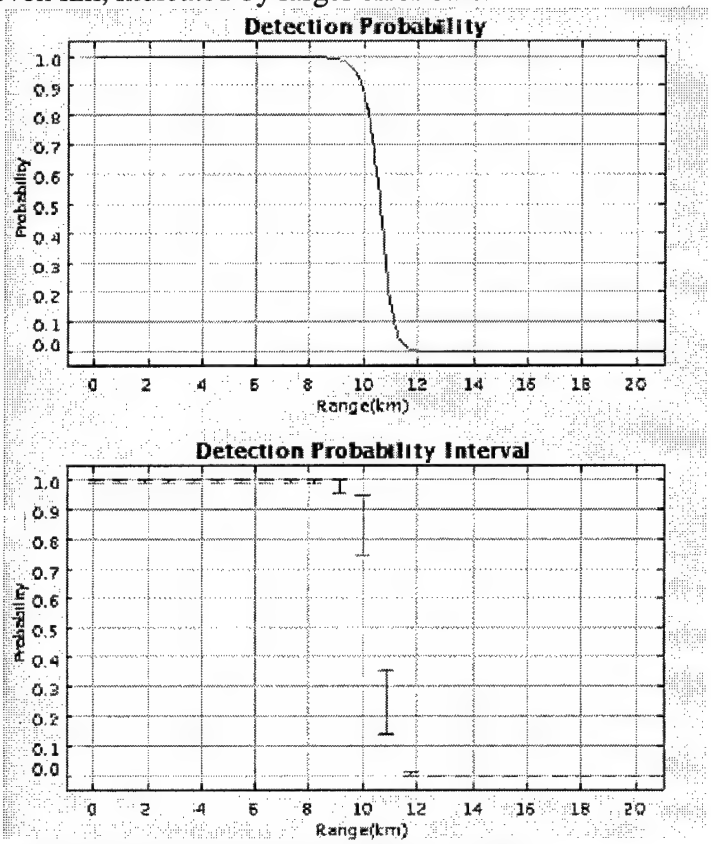

Figure 10. Calculated Detection Probabilities (Soller, 2003)

6.2. Surface Acoustic Wave (SAW) Chemical Sensor Models

6.2.1. A Summary Description of the SAW Detection Process

A SAW sensor exposed to a target gas responds by adsorbing a fraction of the input gas concentration. The gas adsorbed increases the mass of a chemically sensitive coating layer on a piezoelectric substrate. This increased mass will lower the resonance frequency of the piezoelectric resonator controlled oscillator circuit that comprises the chemical detector. In addition, the adsorbed gas can change the mechanical properties of the chemically sensitive (usually polymer) coating layer on the substrate. This also changes the resonant frequency of the circuit.

The output of the SAW detector is the change in frequency of the oscillator/resonator. The change in frequency depends on the type of gas, the concentration of input gas in the chemically-

sensitive layer, and any resultant change in mechanical properties of the chemically sensitive layer. The resulting steady state frequency change is the primary means used to separate input gas mixtures into constituent components.

SAW sensors are observed to reach steady state over a range of times. Similarly, when the target gas is removed, the sensors return to their original states (original resonant frequencies) over a range of times. The attainment of steady state is governed by a combination of adsorption of gas on the surface of the chemically sensitive layer and the diffusion of gas through this layer. Both of these properties depend on the type of polymer used and the target gas.

The clear down or fall time of a chemical sensor depends upon the diffusion of gases out of the sensitive layer and the subsequent desorption of gases from the surface. Desorption is a thermally-activated process, whose activation energy depends upon the interaction energy between the molecules of the sensitive layer and the molecules of the target input gas. These vary for different layers and gases.

The physico/chemical parameters that describe the SAW sensor response are mostly temperature-dependent. The temperature dependence is often complex, and varies depending on sensitive-layer molecules and target gas molecules.

All electronic devices and transducers exhibit fluctuations in their output. These fluctuations exhibit root mean squared (RMS) values and a spectrum of power versus frequency. The noise spectra can be time varying if the mechanisms underlying the noise spectra vary with time. These fluctuations of resonant frequency vary with film geometry, rate of gas adsorption into the film, and fluctuations in transport properties of gas molecules in the film. The fluctuations in transport properties are dependent on the structure and composition of the film.

A detailed analysis of the dynamic response of a SAW sensor or an array of SAW sensors yields information about these operating mechanisms. Different time windows of the device output can be analyzed to understand the impact of these mechanisms on device performance.

6.2.2. Modeling of SAW Detection Process

The investigators developed a model for SAW chemical sensors that incorporated models of the various operating mechanisms. The overall SAW sensor model was implemented as a collection of coupled software components. Each software component represents a model of a single operating mechanism or collection of mechanisms, whose inputs and other parameters are adjustable. By contrast, conventional SAW models are either

- oversimplified or
- make it difficult to implement localized variations in their complex boundary conditions, which include multidimensional relationships.

Conventional SAW models do not readily permit accurate tradeoff analyses for upgrading or adapting detectors to improve the performance of existing detector systems or for responding to new threats.

Over a more limited domain, the models developed in the Phase II research provide the

- the accuracy approaching the more complex models and
- flexibility to support a number of detector-related design and analysis tasks.

Therefore, the component-based modeling approach developed by CogniTech and the University of Utah is more suitable for the analysis and design of SAW and other detector arrays.

The dynamic models were first implemented in the C++ programming language by the University of Utah. The following operating mechanisms were implemented:

1. Adsorption from gas phase to the surface, where Langmuir and Fruendlich isotherms were treated individually
2. Diffusion from the surface into the chemically-sensitive film, where linear (Fickian) diffusion, concentration dependent diffusion, and non-linear diffusion mechanisms were treated individually
3. Desorption from the chemically sensitive film, where transport (diffusion) limited desorption and thermal (interaction energy limited) desorption were treated individually
4. Steady state sensor output, using mass loading (ideal) and mass loading plus changes in viscoelastic properties (non-ideal)
5. Noise spectral density, sometimes called noise floor, based on the sum of noise in a SAW device plus Poisson noise due to adsorption/desorption and transport noise due to diffusion.
6. Dynamic, time-dependent sensor output using
   - diffusion and adsorption mechanisms as enumerated in (1) and (2) for the rise time and
   - diffusion and desorption mechanisms as enumerated in (2) and (3) for the clear down (fall) time.

Parameters and specialized models were identified for various combinations of SAW device configurations (e.g., gases, substrates, chemically-sensitive layers, processing) and atmospheric (e.g., temperatures, pressure, humidity). The outputs of these models were plotted for different polymer substrates and different target gases and shown in figures 11-15. The development of the component-based models, their scientific basis, and their C++ implementation are presented in two recent master's theses at the University of Utah (Cha, 2005; Pandita, 2005).

These models could have been integrated directly from the C++ code or converted to Java components. CogniTech made the decision to re-implement the models in the Java programming language to simplify long-term maintenance of the models. The Java implementation of the SAW models was integrated into the visual drag and drop software environment described in section 5. In this environment, a non specialist in chemical detectors can easily adjust complexity, materials, algorithms, and interconnections in a detector array model to simulate the behavior of array and enable analysis. This represents a significant advance in the analysis, selection, upgrading and adaptation of chemical detectors.

6.2.3. Data Obtained from Component Base Simulations of SAW Sensors

The graphs shown below illustrate typical outputs from the simulation of SAW sensors using the models described in section 6.2.2. Figure 11 shows how steady state is approached after the sensor is exposed to the target gas. The concentration builds up over time until equilibrium is

attained. At equilibrium, adsorption from the gas phase is balanced by desorption to the gas phase. Figure12 shows how the level of fluctuations is minimized in steady state and that a major contributor to the fluctuations is the shot noise associated with adsorption and desorption processes. Figure 13 is the counterpart of figure 11 in the response domain and shows the change in frequency during the adsorption of the target gas. The frequency change with time approaches zero as steady state is attained. Figure 14 shows the dynamic output of the detector for two different gases. It is noteworthy that the rise time differs between the two gases even though the steady state values are comparable. Figure 15 shows the Poisson noise for this detector. As expected, it reaches a minimum at steady state. The zero value refers to the noise in the oscillator that would appear in a saw that wasn't used as a chemical detector.

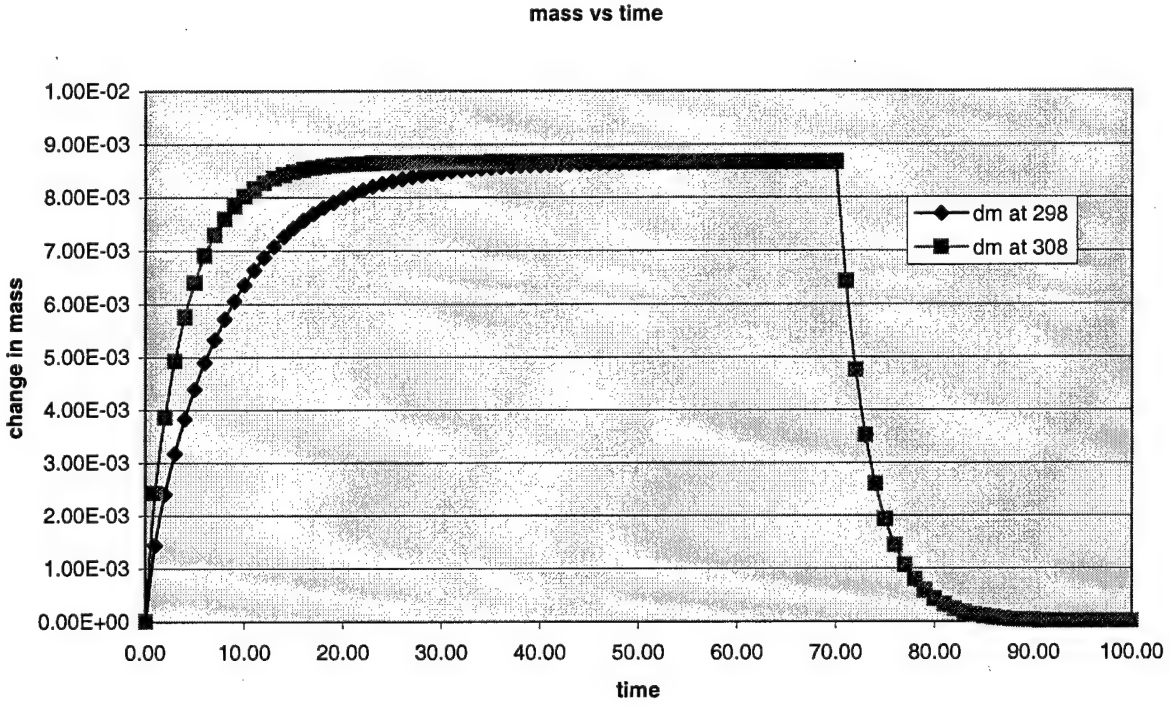

Figure 11. Dynamic Mass Addition and Change in Polymer of Sensor

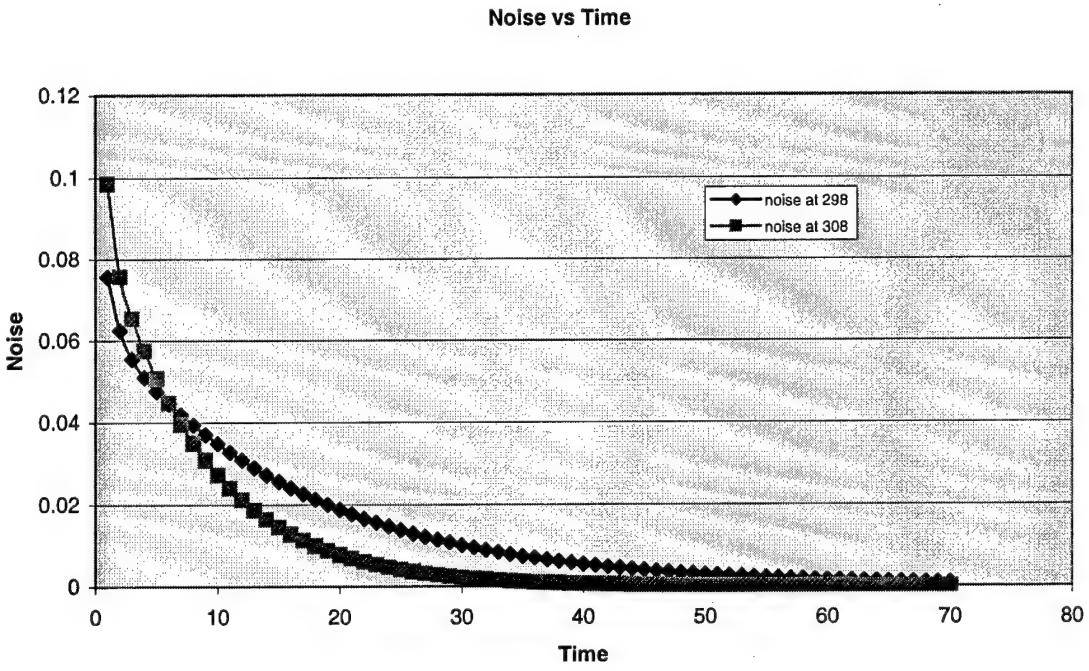

Figure 12. Noise in Sensor Response due to Sorption of Molecules

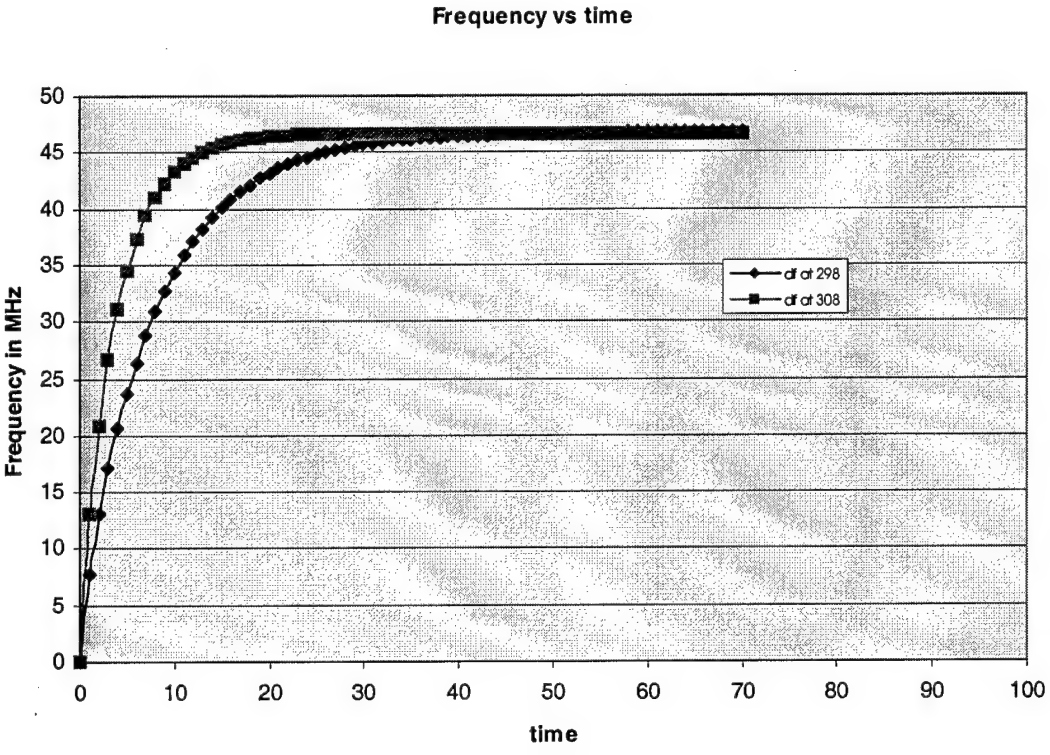

Figure 13. Output Frequency versus Time, Normalized to Resonant Frequency

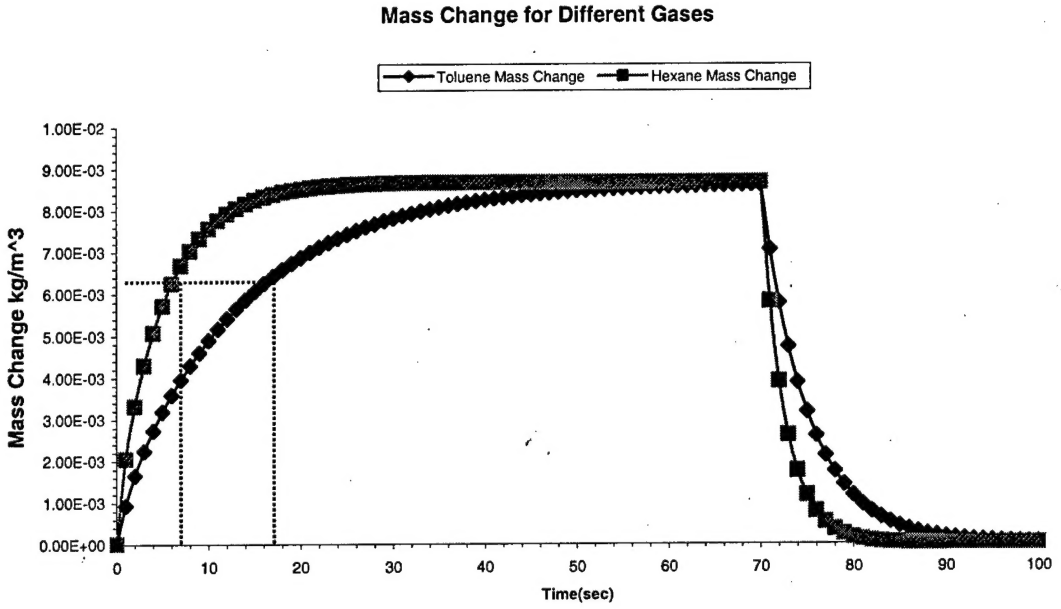

Figure 14. Depiction of Sensor Response for 2 Different Target Gases, Toluene & Hexane

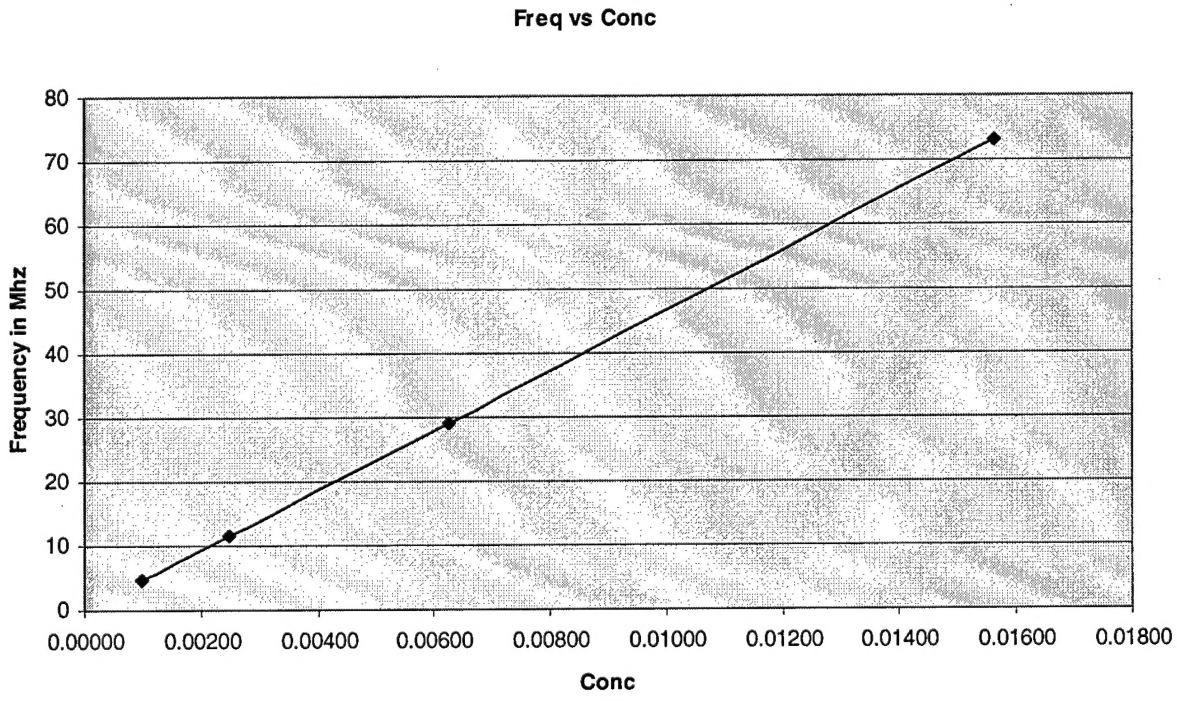

Figure 15. Frequency vs. Concentration Change at Steady State

This research developed the most comprehensive SAW chemical sensor model reported (to our knowledge) in the literature. Specifically, this model provided

- The first scientifically (as opposed to network based) model of a SAW sensor that includes rise time, cleardown time and noise level
- The discovery that a detailed analysis of a SAW sensor output provides much more understanding than the static response, or even the temperature dependent static response.
- Decomposition of SAW output into component contributions permits optimizing a device by determining the impact of proposed changes upon particular parts of the device performance.

6.3. DTRA HPAC

6.3.1 Overview

The Defense Threat Reduction Agency's Hazard Prediction and Assessment Capability (HPAC) computer model (Lee, 2002) uses the atmospheric dispersion model SCIPUFF (Second-order Closure Integrated Puff) as its backend dispersion simulation. SCIPUFF was the first widely accepted vapor dispersion model with an explicit parameterization of model uncertainty.

SCIPUFF uses a Lagrangian puff dispersion model developed by Titan's ARAP Group that uses a collection of Gaussian puffs to represent an arbitrary, three-dimensional time-dependent concentration. The turbulent diffusion parameterization is based on turbulence closure theory, providing a direct relationship between the predicted dispersion rate and turbulent velocity statistics of the wind field. In addition to the average concentration value, the closure model also provides a prediction of the statistical variance in the concentration field resulting from the random fluctuations in the wind field. The closure approach also provides a direct representation for the effect of averaging time.

The principle advantage of the Lagrangian approach, for dispersion modeling, is the absence of any numerical grid, so that the enormous range of scales involved in dispersion from a localized source onto the mesoscale or larger can be accurately represented .

HPAC includes the ability to interface with several meteorological data servers in addition to the ability to accept data from larger scale meteorology simulations such as MM5. HPAC also models dense gas behavior and includes the ability to specify linear decay rates for any species.

6.3.2 Software Interface

HPAC was chosen as the demonstration vapor dispersion model because it already has external CORBA interfaces available. With the assistance of DTRA staff, SAIC and Oak Ridge National Laboratory, CogniTech developed a simulation module for use within the sensor simulation environment using the HPAC dispersion engine. This module invokes the HPAC software running on the same or a remote system to operate on previously configured scenarios and return the simulation data. The module was written in the Java programming language and tested with both stand-alone and distributed configurations. The HPAC software itself must be run on a Microsoft Windows platform, but may be invoked from the CogniTech client running on any platform that supports Java (e.g. Windows, Linux, Unix).

7. Conclusion

The research performed in this Phase II SBIR contract developed a generalized architecture, framework, and methodology for the modeling and simulation of chemical and biological (CB) detectors. The software environment integrates atmospheric models, detector models, uncertainty measures, and a variety of time-synchronization and model composition capabilities. This framework provides distributed access to models and simulations. Simulation components were developed for standoff and point detectors, including the most complete dynamic model of the Surface Acoustic Wave (SAW) chemical sensor to date.

The data resulting from the simulations enabled analysis of various detector capabilities and tradeoffs using multiple metrics. Future directions include the development and integration of an enhanced environment; more comprehensive suite of sensor models; a database for experimental and simulated data; sensor data interpretation algorithms; and data fusion to support seamless modeling, design, testing, and analysis for current and future chemical and biological detection assets. In addition, this technology can serve as the foundation for a sensor simulation capability to be integrated with DoD atmospheric hazard dispersion models and an interface to decision support systems.

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